

Topological Change of the Fermi Surface in Low Density Rashba Gases: Application to Superconductivity

E. Cappelluti^{1,2}, C. Grimaldi^{3,4}, and F. Marsiglio^{4,5}

¹*SMC-INFM and Istituto dei Sistemi Complessi,*

CNR-INFM, via dei Taurini 19, 00185 Roma, Italy

²*Dipart. di Fisica, Università "La Sapienza", P.le A. Moro 2, 00185 Roma, Italy*

³*LPM, Ecole Polytechnique Fédérale de Lausanne, Station 17, CH-1015 Lausanne, Switzerland*

⁴*DPMC, Université de Genève, 24 Quai Ernest-Ansermet, CH-1211 Genève 4, Switzerland and*

⁵*Department of Physics, University of Alberta, Edmonton, Alberta, Canada, T6G 2J1*

Strong spin-orbit coupling can have a profound effect on the electronic structure in a metal or semiconductor, particularly for low electron concentrations. We show how, for small values of the Fermi energy compared to the spin-orbit splitting of Rashba type, a topological change of the Fermi surface leads to an effective reduction of the dimensionality in the electronic density of states. We investigate its consequences on the onset of the superconducting instability. We show, by solving the Eliashberg equations for the critical temperature as a function of spin-orbit coupling and electron density, that the superconducting critical temperature is significantly tuned in this regime by the spin-orbit coupling. We suggest that materials with strong spin-orbit coupling are good candidates for enhanced superconductivity.

PACS numbers: 72.25.-b, 72.10.-d, 72.20.Dp

Spin-orbit (SO) coupling arising from the lack of inversion symmetry plays a leading role in the field of spintronics [1]. One of the main goals in this field of research is the possibility of tuning the electron spin properties (transport, coherence, relaxation, etc.) by means of electrical fields [2]. With this aim in mind, different properties have been investigated, such as spin relaxation [3], magnetoconductance [4] and spin-Hall currents [5]. As a general rule, the spin-orbit coupling is assumed to be quite small with respect to the other relevant energy scales, in particular with respect to the electronic dispersion, so that the infinite bandwidth limit is often employed. While this assumption is indeed rather reasonable in most of the cases, the natural aim of the current investigations is to search for new materials with stronger spin-orbit couplings, as for instance in HgTe quantum wells [6], or the surface states of metals and semimetals [7, 8]. For this reason, experimental evidence of a Rashba SO coupling with energy E_0 (to be defined below) as large as $\simeq 220$ meV in bismuth/silver alloys [9], or with $E_0 \simeq 30 - 200$ meV in non-centrosymmetric superconductors CePt₃Si [10, 11], Li₂Pd₃B, and Li₂Pt₃B [12, 13], is certainly an important step towards the investigation of new materials with large SO coupling. Needless to say, the existence of such materials compels us to carry out a more thorough investigation of the properties of SO systems when E_0 is no longer necessarily the smallest energy scale in the problem.

The possibility of having novel interesting features in low density systems with Fermi energy E_F of the same order or lower than the SO energy E_0 , in particular, has not been sufficiently investigated to date, in our opinion, and only few studies have been devoted to this problem. In Ref. [14] for instance, it was shown that the vanishing

of the spin-Hall current in the low density limit $n \rightarrow 0$ of Rashba disordered systems is not related to the vanishing of the vertex function (which applies only in the strict $E_F/E_0 \rightarrow \infty$ limit) but rather to the cancellation between on-Fermi surface and off-Fermi surface contributions. Another interesting effect was also pointed out in Ref. [15]: there the spin relaxation time τ_s for $E_F \ll E_0$ was shown to be proportional to the electron scattering time τ , in contrast with the standard Dyakonov-Perel behavior, where τ_s scales as $1/\tau$ [16]. On the other hand, in spite of the growing interest in the properties of non-centrosymmetric superconductors with strong SO coupling [17, 18], no specific investigation to explore the regime where $E_F/E_0 \lesssim 1$ has been pursued, to our knowledge.

The aim of this Letter is to explore in detail a fundamental feature arising in SO Rashba systems, namely the topological change of the Fermi surface induced by the strong SO interaction in the low density regime $E_F/E_0 \leq 1$. We show that in this situation the enhanced phase space available for the electronic excitations gives rise to a SO-induced change of the electronic density of states which can be described in terms of an effective reduced dimensionality. We discuss the consequences of this scenario on the superconducting instability criterion for both two- and three-dimensional Rashba systems. We show that, in contrast with the high density case $E_F/E_0 \gg 1$, the SO coupling in the $E_F/E_0 \lesssim 1$ regime systematically enhances the superconducting critical temperature T_c , providing evidence that the lack of inversion symmetry can be remarkably beneficial for superconducting pairing.

We begin our analysis by considering the Rashba model [19] which describes the linear coupling of conduction

electrons with a spin-orbit potential of the form

$$\gamma(k_x\sigma_y - k_y\sigma_x), \quad (1)$$

where σ_x, σ_y are Pauli matrices and γ is the Rashba coupling constant. For two-dimensional systems such as asymmetric quantum wells and surface states of metals and semimetals the SO coupling in Eq. (1) arises from the asymmetric confining potential, while in bulk three-dimensional compounds Eq. (1) originates from the lack of reflection symmetry with respect to the z -direction, as in CePt₃Si. The SO coupling is reflected in an energy splitting of the two helicity bands. Assuming a parabolic band for $\gamma = 0$, the resulting dispersion of the electronic excitations, for two-dimensional (2D) and three-dimensional (3D) cases, reduces to

$$E_{\pm}^{2D}(k) = \frac{\hbar^2}{2m^*} (k \pm k_0)^2, \quad (2)$$

$$E_{\pm}^{3D}(k) = \frac{\hbar^2}{2m^*} (k \pm k_0)^2 + \frac{\hbar^2 k_z^2}{2m^*}, \quad (3)$$

where $k = |\mathbf{k}|$ is the modulus of the xy in-plane momentum $\mathbf{k} = (k_x, k_y)$, k_z is the wavevector along the z -direction, and m^* is the effective electron mass. In addition $k_0 = m^*\gamma/\hbar^2$ represents here the characteristic Rashba momentum. The dispersion for the 2D case is shown in Fig. 1a, which can easily be generalized in the 3D case by taking into account the k_z dispersion. The two horizontal dashed lines correspond to the Fermi level for high density and low density regimes defined as $E_F > E_0$ and $E_F < E_0$ respectively, where $E_0 = \hbar^2 k_0^2 / 2m^*$ is the energy of the $\mathbf{k} = 0$ point with respect to the bottom band edge at $k = k_0$ (see Fig. 1a).

Density of states - Several studies in the literature have focused on the high density regime, $E_F \gg E_0$, where the two Fermi surfaces belong to different helicity bands, and where the Fermi volume V_F is given by the area of two concentric Fermi circles $V_F = \pi k_{F,+}^2 + \pi k_{F,-}^2$ with $k_{F,\pm} = \sqrt{2m^*/\hbar^2} (\sqrt{E_F} \mp \sqrt{E_0})$. In this case the electronic density of states (DOS) at the Fermi level is given by

$$N^{2D}(E_F) = \sum_s \frac{1}{4\pi^2} \int_{S_{F,s}} \frac{dS_k}{\hbar |v_{k,s}|} = \sum_s \frac{1}{4\pi^2 \hbar} \frac{S_{F,s}}{|v_{F,s}|}, \quad (4)$$

where the Fermi velocity $|v_{F,\pm}| = \sqrt{2E_F/m^*}$ is independent of the helicity number $s = \pm$ and the Fermi surfaces are $S_{F,\pm} = 2\pi k_{F,\pm}$. Hence the total DOS in the $E_F > E_0$ regime $N^{2D}(E_F) = m^*/(\pi\hbar^2)$ is identical to the one in the absence of spin-orbit coupling. A similar result applies for the 3D case where, from Eq. (3), the corresponding DOS can be obtained as

$$N^{3D}(E_F) = \int \frac{dk_z}{2\pi} N^{2D}(E_F - \hbar^2 k_z^2 / 2m^*). \quad (5)$$

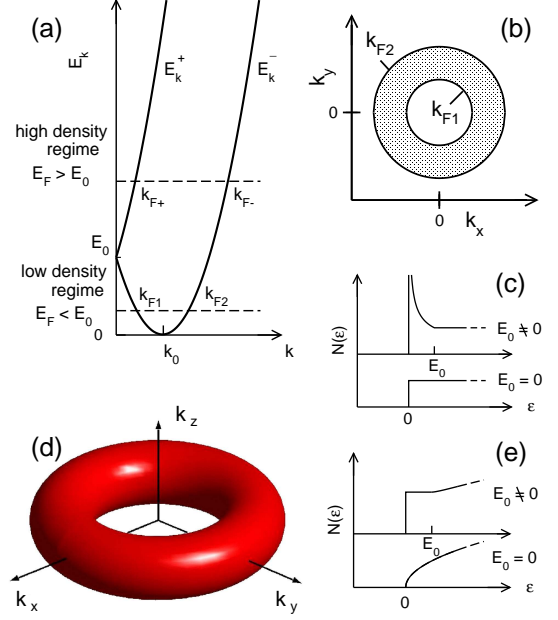


FIG. 1: Panel (a): electronic dispersion in the presence of SO coupling: for $E_F \geq E_0$ (high density regime) the two Fermi surfaces belong to different helicity bands, while for $E_F \leq E_0$ (low density regime) the Fermi surface exists only on the E_k^- band. Also shown here is the Rashba energy E_0 corresponding to the lowest interband excitation energy for an electron lying at the bottom of the lower band. Panels (b) and (c): Fermi surface and density of states, respectively, in the low density regime for the two-dimensional case. Panels (d) and (e): Fermi surface and density of states in the low density regime for the three-dimensional case.

In the high density regime $E_F \geq E_0$ we get $N^{3D}(E_F) = a\{\sqrt{E_F - E_0} + \sqrt{E_0} \arctan[\sqrt{E_0/(E_F - E_0)}]\}$, where $a = \sqrt{2m^*}^{3/2}/(\pi^2 \hbar^3)$, which reduces to $N^{3D}(E_F) \simeq a\sqrt{E_F}$ in the $E_F/E_0 \gg 1$ limit. This again is the result one obtains in the absence of SO coupling.

Let us now consider the $E_F \leq E_0$ regime. In this case the Fermi level intersects only the lower $E_-(k)$ band and the topology of the Fermi surfaces drastically changes. In the 2D case for instance only the annulus that lies between two Fermi circles of radii $k_{F,2} = \sqrt{2m^*/\hbar^2} (\sqrt{E_0} + \sqrt{E_F})$ and $k_{F,1} = \sqrt{2m^*/\hbar^2} (\sqrt{E_0} - \sqrt{E_F})$, belonging to the *same* helicity band, is filled (Fig. 1b), and the inner Fermi surface is *inwards* oriented. We can still employ Eq. (4) by summing over the two Fermi surface indexes $s = 1, 2$. Using $|v_{F,s}| = \sqrt{2E_F/m^*}$ and $S_{F,s} = 2\pi k_{F,s}$ we get

$$N^{2D}(E_F) = \frac{m^*}{\pi \hbar^2} \sqrt{\frac{E_0}{E_F}}, \quad (6)$$

which is valid as long as $E_F \leq E_0$ (Fig. 1c). Most peculiar is the square-root divergence for $E_F \rightarrow 0$ that is reminiscent of one-dimensional behavior. We relate such

a feature to the non-vanishing in the low density limit of the Fermi surface which remains finite, $S_{F,s} \propto \sqrt{E_0}$, while at the same time, the Fermi velocity vanishes as $\sqrt{E_F}$. The behavior of Eq. (6) has to be compared with the $\gamma = 0$ case where also the Fermi surface shrinks as $\sqrt{E_F}$ and the electron DOS has a non divergent step-like behavior in the $E_F \rightarrow 0$ limit [20].

A similar reduction of effective dimensionality in the electron DOS appears also for the 3D systems in the $E_F \leq E_0$ regime. In this case the Fermi surface has a torus-like topology as shown in Fig. 1d, with major radius $k_0 = \sqrt{2m^*E_0/\hbar^2}$ and minor radius $\sqrt{2m^*E_F/\hbar^2}$. Applying once more Eq. (5) we get

$$N^{3D}(E_F) = \frac{\pi a}{2} \sqrt{E_0}, \quad (7)$$

for $E_F \leq E_0$. We see therefore that the SO coupling changes qualitatively the low density behavior of the DOS providing a finite step-like behavior (Fig. 1e) in contrast with a standard 3D electron gas whose DOS vanishes as $\sqrt{E_F}$.

Cooper instability - The above described reduction of effective dimensionality sheds a new light on the possible existence of a superconducting phase in the low density regime of systems with no inversion symmetry. To illustrate this point let us consider the classical problem [21] of a Fermi surface instability towards the formation of a Cooper pair:

$$1 = V \int_0^{\omega_0} d\xi N(\xi) \frac{1}{2\xi + \Delta}, \quad (8)$$

where $\Delta > 0$ is the binding energy of the bound pair state, V is the strength of the interaction which we consider here for simplicity in the s -wave channel, and where we have introduced a standard BCS cut-off ω_0 related to the energy of the underlying bosonic mediator. Since the superconducting Cooper pairing is essentially a Fermi surface instability, the strength of the bound state and its existence itself is intimately related to the phase space of the available electronic excitations. For instance, as well known, in the low density limit of 3D systems, where $N^{3D}(\xi) = a\sqrt{\xi}$, Eq. (8) predicts a finite critical coupling $V_c = 1/(a\sqrt{\omega_0})$ below which no bound state exists.

This result changes drastically for finite SO couplings where, as seen above, the electron DOS behaves now as an effective 2D system with a constant value in the low energy regime. Using Eq. (7) in Eq. (8) we get:

$$\Delta_{3D} \simeq 2\omega_0 \exp\left(-\frac{4}{\pi a V \sqrt{E_0}}\right), \quad (9)$$

which explicitly shows that, contrary to the usual 3D case, the Cooper pair instability exists no matter how weak V is. Furthermore Eq. (9) predicts that the pair energy Δ has an exponential dependence on the SO coupling, as is normally the case (here as well) for the attractive potential.

A similar change of the character of the Cooper instability occurs also in the 2D case. Indeed, in the absence of SO coupling, one would get the standard BCS result $\Delta = 2\omega_0 \exp(-2\pi\hbar^2/m^*V)$. On the other hand, due to the strong one-dimensional-like divergence of the electron DOS, Eq. (6), the binding energy for finite SO coupling reads now

$$\Delta_{2D} = \frac{1}{2} \left(\frac{m^*V}{\hbar^2} \right)^2 E_0, \quad (10)$$

where the bosonic energy ω_0 is no longer present and the relevant energy scale is provided by E_0 . Note also the quadratic dependence of the binding energy Δ with respect to the coupling strength V , and the complete absence of an isotope effect for the phonon-mediator case.

Superconducting critical temperature - The above discussion of the single Cooper pair problem will be now a guide to the following investigation of the superconducting transition for finite (low) densities in fully interacting systems. To this end we consider a Rashba-Holstein model where the SO coupled electrons interact with dispersionless bosons with energy ω_0 through an s -wave coupling with matrix element g [22]. The superconducting properties, and in particular the critical temperature T_c , are evaluated within the Eliashberg framework properly generalized in the presence of SO coupling, with general values of E_F/E_0 , including the low density case just discussed. Note that due to the lack of inversion symmetry, a different superconducting phase with mixed even/odd order parameter and singlet/triplet symmetry can in principle be included [18]. We neglect here for simplicity this issue and focus only on the s -wave singlet channel.

In Fig. 2a,c we show the superconducting critical temperature T_c as a function of the SO Rashba energy E_0 for different electron densities n . In the figure the lower density values, $n = 10^{13} \text{ cm}^{-2}$ and $n = 10^{20} \text{ cm}^{-3}$, correspond to Fermi energies $E_F \simeq 24 \text{ meV}$ and $E_F \simeq 46 \text{ meV}$ for the free electron gas in 2D and 3D respectively. In addition, for a practical purpose one needs to introduce a finite bandwidth cut-off E_c , which is physically provided by the size of the Brillouin zone k_c . We set $E_c = 2000(430) \text{ meV}$ which give $k_c \simeq 0.72(0.33) \text{ \AA}^{-1}$ respectively for the 2D and 3D case. We get thus an energy-dimensional electronic DOS per unit cell which, for the density values reported above in the absence of SO coupling, is $N_{2D}(E_F = 24 \text{ meV}) \simeq 5 \cdot 10^{-4} \text{ meV}^{-1}$ and $N_{3D}(E_F = 46 \text{ meV}) \simeq 12 \cdot 10^{-4} \text{ meV}^{-1}$. For all cases ω_0 has been fixed at $\omega_0 = 20 \text{ meV}$ and $g = 5\omega_0$. With these values we obtain dimensionless coupling constants $\lambda = 2g^2 N(E_F)/\omega_0$ respectively $\lambda_{2D}(E_F = 24 \text{ meV}) \simeq 0.5$ and $\lambda_{3D}(E_F = 46 \text{ meV}) \simeq 0.6$. Fig. 2a,c shows a significant increase of T_c as a function of E_0 , in particular for low densities where a small E_0 is sufficient to enter into the $E_F \lesssim E_0$ regime. This holds true for both 2D and 3D systems, and the enhancement of T_c can be as high as

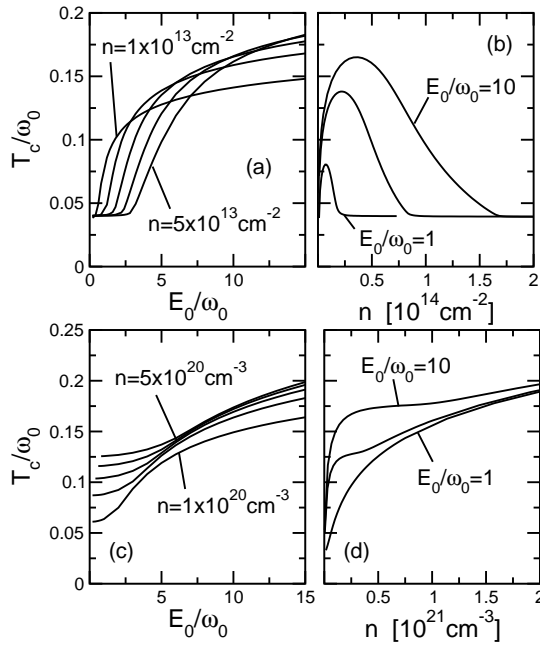


FIG. 2: Panels (a) and (b): Superconducting critical temperature T_c as function of the Rashba spin-orbit energy E_0 and of the electron density n , respectively, for the 2D case. Panels (c) and (d): same quantities for the 3D system.

300 % with respect to the $E_0 \rightarrow 0$ limit. Also interesting is the study of the superconducting critical temperature as a function of the electron density n , as reported in Fig. 2b,d. In these panels it is evident how the T_c vs. n behavior reflects the effective dimensionality reduction of the underlying non interacting DOS. For example for the 2D case T_c is nearly constant as a function of electron density for $E_0 = 0$; this is consistent with the constant electron DOS. In contrast, for finite E_0 the presence of strong peaks in T_c vs. n reflects the 1D-like singularity of the DOS. Note however that the retarded electron-boson interaction gives rise to dynamical one-particle renormalization effects, automatically taken into account in the Eliashberg equations, which smear the singularity of the bare DOS.

Similarly, in the $E_0 \rightarrow 0$ limit of the 3D case T_c drops as the density n is reduced due to vanishing of $N_{3D}(E_F) \propto \sqrt{E_F}$. On the other hand the 2D character of the DOS with $E_0 \neq 0$ gives rise to an almost flat dependence of T_c for sufficiently low n , with a critical temperature tuned by the Rashba energy E_0 . Both the 2D and 3D case thus show that the lack of inversion symmetry not only affects the character of the order parameter, as discussed in several works [11, 17, 18], but in principle can also lead to a substantial enhancement of the superconducting pairing in the low density regime. As explained above, this phenomenon is triggered by the topological change of the Fermi surface due to the strong

SO interaction.

Let us discuss now the relevance of our results in the context of real materials. Concerning the 2D case, for instance, surface states and low dimensional heterostructures could be natural candidates for the search of enhanced superconductivity. In particular the issue of surface superconductivity [23] has recently been brought to attention due to its relevance for systems like alkali-doped WO_3 [24] where, for sufficiently low concentrations of the alkali atoms, evidence of superconductivity confined to the surface has been provided; this is precisely where strong SO coupling arises from the confinement of the surface potential. Interesting perspectives are also given by the non-centrosymmetric superconductors, such as CePt_3Si , $\text{Li}_2\text{Pd}_3\text{B}$, and $\text{Li}_2\text{Pt}_3\text{B}$, where a strong Rashba energy arises from the lack of inversion symmetry in the bulk crystal. In the $\text{Li}_2\text{Pd}_3\text{B}$ and $\text{Li}_2\text{Pt}_3\text{B}$ compounds, in particular, a large SO coupling is accompanied by a strong electron-phonon interaction [25]. In this case, of course, as in the heavy fermion CePt_3Si case, a proper generalization of the present results to the case of non parabolic bands is needed.

In summary, we have examined the impact of a strong Rashba spin-orbit interaction on superconductivity in a weakly coupled electron-boson system. The primary result is an effective reduction in dimensionality of the electronic density of states. This accomplishes what the Fermi sea did for the Cooper pair problem in 3 dimensions — it increased phase space at the Fermi level significantly to allow binding for arbitrarily weak interactions. We then performed full Eliashberg calculations of the critical temperature for a wide range of parameters; these illustrate that the enhanced density of states has a significant impact on the superconducting critical temperature. We suggest a search for higher critical temperatures in materials with large spin-orbit coupling. In systems where electron density can be varied one should be able to test some of the trends reported here.

This work was supported in part by the Natural Sciences and Engineering Research Council of Canada (NSERC), by ICORE (Alberta), by the Canadian Institute for Advanced Research (CIAR), and by the University of Geneva.

-
- [1] S. A. Wolf, D. D. Awschalom, R. A. Buhrman, J. M. Daughton, S. von Molnár, M. L. Roukes, A. Y. Chtchelkanova, and D. M. Treger, *Science* **294**, 1488 (2001).
 - [2] P. Sharma, *Science* **307**, 531 (2005).
 - [3] I. Žutić, J. Fabian, and S. Das Sarma, *Rev. Mod. Phys.* **76**, 323 (2004).
 - [4] P. Schwab and R. Raimondi, *Eur. Phys. J. B* **25**, 483 (2002).
 - [5] H.-A. Engel, E.I. Rashba, and B.I. Halperin,

- cond-mat/0603306; J. Schliemann, *Int. J. Mod. Phys. B* **20**, 1015 (2006).
- [6] Y. S. Gui, C.R. Becker, N. Dai, J. Liu, Z.J. Qiu, E.G. Novik, M. Schafer, X.Z. Shu, J.H. Chu, H. Buhmann, and L.W. Molenkamp, *Phys. Rev. B* **70**, 115328 (2004)
 - [7] E. Rotenberg, J. W. Chung, and S. D. Kevan, *Phys. Rev. Lett.* **82**, 4066 (1999).
 - [8] Yu. M. Koroteev, G. Bihlmayer, J. E. Gayone, E. V. Chulkov, S. Blugel, P. M. Echenique, and P. Hofmann, *Phys. Rev. Lett.* **93**, 046403 (2004).
 - [9] C.R. Ast, D. Pacile, M. Falub, L. Moreschini, M. Pagnano, G. Wittich, P. Wahl, R. Vogelgesang, M. Grioni, K. Kern, cond-mat/0509509 (2005).
 - [10] E. Bauer, G. Hilscher, H. Michor, Ch. Paul, E. W. Scheidt, A. Griбанov, Yu. Seropegin, H. No"el, M. Sigrist, and P. Rogl, *Phys. Rev. Lett.* **92**, 027003 (2004).
 - [11] K. V. Samokhin, E. S. Zijlstra, and S. K. Bose, *Phys. Rev. B* **69**, 094514 (2004).
 - [12] K. Togano, P. Badica, Y. Nakamori, S. Orimo, H. Takeya, and K. Hirata, *Phys. Rev. Lett.* **93**, 247004 (2004).
 - [13] H.Q. Yuan, D.F. Agterberg, N. Hayashi, P. Badica, D. Vandervelde, K. Togano, M. Sigrist, and M. B. Salamon, *Phys. Rev. Lett.* **97**, 017006 (2006).
 - [14] C. Grimaldi, E. Cappelluti, and F. Marsiglio, *Phys. Rev. B* **73**, 081303(R) (2006).
 - [15] C. Grimaldi, *Phys. Rev. B* **72**, 075307 (2005).
 - [16] M.I. Dyakonov and V.I. Perel, *Fiz. Tverd. Tela* (Leningrad) **13**, 3581 (1971) [*Sov. Phys. Solid State* **13**, 3023 (1971)].
 - [17] L.P. Gor'kov and E.I. Rashba, *Phys. Rev. Lett.* **87**, 037004 (2001).
 - [18] P.A. Frigeri, D.F. Agterberg, A. Koga, and M. Sigrist, *Phys. Rev. Lett.* **92**, 097001 (2004).
 - [19] E.I. Rashba, *Sov. Phys. Solid State* **2**, 1224 (1960).
 - [20] Systems with minimum dispersion at $k_0 \neq 0$, and therefore with a square root divergence of the corresponding DOS, have been recently discussed in K. Yang and S. Sachdev, *Phys. Rev. Lett.* **96**, 187001 (2006), within the context of quantum criticality of unbalanced species of paired fermions.
 - [21] L.N. Cooper, *Phys. Rev.* **104**, 1189 (1956).
 - [22] C. Grimaldi, E. Cappelluti, and F. Marsiglio, *Phys. Rev. Lett.* **97**, 066601 (2006).
 - [23] L.P. Gor'kov, *Int. J. Mod. Phys. B* **20**, 2569 (2006).
 - [24] Y. Levi, O. Millo, A. Sharoni, Y. Tsabba, G. Leituss, and S. Reich, *Europhys. Lett.* **51**, 564 (2000).
 - [25] K.W. Lee and W.E. Pickett, *Phys. Rev. B* **72**, 174505 (2005).